

ABSTRACT

A catalyst development engine (CDE) provides a rapid approach to the rational development of scalable heterogeneous catalysts and of high-performance solid materials. The CDE includes three main components: the testing cycle, the knowledge cycle, and the knowledge repository or database. The knowledge cycle generates working hypotheses relating performance to key catalyst properties via machine learning methods, computation chemistry and micro-kinetic modeling. Such an approach accelerates development and scale-up of new materials without the impediments introduced by conventional combinatorial approaches based on randomly selected materials.

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